Swelling-Collapse Transition of Self-Attracting Walks

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We study the structural properties of self-attracting walks in d dimensions using scaling arguments and Monte Carlo simulations. We find evidence for a transition analogous to the Θ transition of polymers. Above a critical attractive interaction u_c, the walk collapses and the exponents ν and k, characterising the scaling with time t of the mean square end-to-end distance $\langle R^2 \rangle \sim t^{2\nu}$ and the average number of visited sites $\langle S \rangle \sim t^k$, are universal and given by $\nu = 1/(d+1)$ and $k = d/(d+1)$. Below u_c, the walk swells and the exponents are as with no interaction, i.e. $\nu = 1/2$ for all d, $k = 1/2$ for $d = 1$ and $k = 1$ for $d \geq 2$. At u_c, the exponents are found to be in a different universality class.

In recent years different models of random walks with memory or interaction have been studied. They can be divided in static [1] and dynamic [2,3] models, for an overview we refer to the papers of Duxbury and Queiroz [1] and Oettinger [2]. Most efforts concentrated on models with repulsive interactions, in particular self-avoiding walks (SAW), which have been found useful for investigating polymers in dilute solution. When an attraction term $\exp(-A/T)$, $A<0$, is included, the SAW model reveals a swelling-collapse transition at the 'Θ point' $T=\Theta$ [4,5]. In contrast, the likewise challenging case of random walks with a similar attractive interaction, but without repulsion, has been less understood. This problem was solved only for one dimension, while in higher dimensions the results are highly controversial. Our numerical and analytical study of attractive random walks suggests that there exists a swelling-collapse transition, too, that is analogous to the Θ transition in polymers.

We focus on the dynamic model of self-attracting walks ($SATW$) [3], where a random walker jumps with probability $p \sim \exp(nu)$ [6] to a nearest neighbor site, with $n=1$ for already visited sites and $n=0$ for not visited sites. The interaction parameter u is equivalent to $-A/T$ for linear polymers. For $u>0$, the walk is attracted to its own trajectory [7]. The structural behavior of the walk can be characterized by the mean square end-to-end distance $\langle R^2(t)\rangle$ and the average number of visited sites $\langle S(t)\rangle$. It is expected that these quantities scale with time t as

$$\langle R^2(t)\rangle \sim t^{2\nu} \tag{1a}$$

and

$$\langle S(t)\rangle \sim t^{k}\ . \tag{1b}$$

Earlier analyses for the $SATW$ in two and three dimensions were not conclusive and the numerical data have been controversially interpreted [3,8–10]. While Sapozhnikov [3] considered the possibility of the existence of a critical attraction u_c (but his numerical results were not conclusive), Lee [8] and Reis [9] argue strongly against the existence of u_c, since they find ν and k continuously decreasing with u.

In this Letter we present scaling arguments and extensive numerical simulations for $\langle R^2\rangle$ and $\langle S\rangle$ that strongly suggest the existence of a critical attraction u_c in $d\geq 2$, with three different universality classes for $u>u_\mathrm{c}$, $u<u_\mathrm{c}$ and $u=u_\mathrm{c}$. Below u_c, the $SATW$ is in the universality class of random walks, with $\nu=1/2$ and $k=1$. Above u_c, the $SATW$ collapses and the exponents change to $\nu=1/(d+1)$ and $k=d/(d+1)$. At the critical point, the exponents are $\nu_\mathrm{c}=0.40\pm0.01$ and $k_\mathrm{c}=0.80\pm0.01$ in $d=2$ and $\nu_\mathrm{c}=0.32\pm0.01$ and $k_\mathrm{c}=0.91\pm0.03$ in $d=3$ [11]. The existence of u_c is in striking similarity to the 'Θ point' phenomenon of linear polymers [4,5] where three different universality classes for $T>\Theta$, $T=\Theta$ and $T<\Theta$ exist.

We used Monte-Carlo simulations to study $\langle R^2(t)\rangle$ and $\langle S(t)\rangle$. Figure 1 shows representative results of $\langle R^2(t)\rangle$, for several values of u in $d=3$. For large values of u, the curves bend down towards the slope of $2\,\nu\cong0.5$, while for small values of u, the curves bend up towards the slope of $2\,\nu\cong1$. At some intermediate critical value $u_\mathrm{c}\cong1.9$, the slope is approximately $2\,\nu_\mathrm{c}\cong0.64$. The mean number of visited sites $\langle S(t)\rangle$ shows similar behavior, with $k\cong1$ below u_c, $k_\mathrm{c}\cong0.91$ at u_c, and $k\cong0.75$ above u_c. Figure 2a summarizes the asymptotic exponents ν and k as a function of u in $d=3$. We obtained similar results in $d=2$, the asymptotic values of ν and k are presented in Fig. 2b. In Table I the values of the exponents are summarized and compared with the analogous known exponents for the Θ transition in linear polymers.

In the following we present analytical arguments for the exponents above criticaltity, which can explain our numerical findings. We assume that for sufficiently strong attraction $u>u_\mathrm{c}$ the grown clusters are compact, so that the average number of visited sites scales with the rms displacement $\langle R(t)\rangle \equiv \langle R^2(t)\rangle^{1/2}$ as

$$\langle S(t)\rangle \sim \langle R(t)\rangle^{d}, \qquad u \gg u_\mathrm{c}. \tag{2}$$

Comparing Eq. (1) and Eq. (2) yields

$$k=\nu d, \qquad\qquad u\gg u_\mathrm{c}. \tag{3}$$

For sufficiently strong attraction it takes a very long time for the walker to jump to an unvisited site. Before doing this, the walker diffuses around on the visited sites, being located with equal probability on any of the cluster sites. Hence the mean cluster growth rate is proportional to the ratio between the number of boundary sites and the total number of the cluster sites [3,12]:

$$\frac{\mathrm{d}\langle S\rangle}{\mathrm{d}t} \sim \frac{\langle R\rangle^{d-1}}{\langle R\rangle^{d}} \sim t^{-\nu}. \tag{4}$$

Thus $\langle S\rangle \sim t^{-\nu+1}$. Combining this result with Eq. (1b) and (3), we obtain

$$\nu = \frac{1}{d+1} \tag{5a}$$

and

$$k = \frac{d}{d+1} \tag{5b}$$

for $u \gg u_{\rm c}$.

Because of universality we assume that these results, which are in agreement with the exact values $\nu = 1/2$ and $k = 1/2$ in $d = 1$ [10] and are supported by our extensive Monte Carlo simulations in $d = 2$ and $d = 3$, are valid for all $u > u_{\rm c}$. Indeed, Fig. 2 suggests that the predictions for $u > u_{\rm c}$ (Eq. (5)) are approached asymptotically. We like to note that in $d = 2$ the relation $k = \nu d$ also holds for $u \leq u_{\rm c}$, while in $d = 3$ the numerical results yield $k < \nu d$ for $u < u_{\rm c}$. Since the mass of the generated clusters scales like $M \sim S \sim R^{k/\nu}$, k/ν corresponds to the fractal dimension $d_{\rm f}$ of the cluster. In $d = 2$ the clusters are compact for all u as $k/\nu = d_{\rm f} = d$. In $d = 3$ they are compact for $u > u_{\rm c}$, while for $u < u_{\rm c}$, the fractal dimension of clusters generated by simple random walks $d_{\rm f} = 2 < d$ is obtained. At the criticality, we find $d_{\rm f} = 2.84 \pm 0.25$, but we cannot rule out the possibility that $d_{\rm f} = d$.

To understand the behavior in the critical regime we suggest the following scaling approach. Guided by Fig. 1, we assume that there exists a crossover time t_ξ below which the exponent ν is close to $\nu_{\rm c}$ and above which ν approaches $1/2$ for $u < u_{\rm c}$ and $1/(d+1)$ for $u > u_{\rm c}$. This suggests the following scaling relations:

$$R(t) \sim t^{\nu_{\rm c}} f_\pm(t/t_\xi) \tag{6a}$$

and

$$S(t) \sim t^{k_{\rm c}} g_\pm(t/t_\xi)\ , \tag{6b}$$

where

$$t_\xi = |u - u_{\rm c}|^{-\alpha}\ . \tag{6c}$$

The plus sign refers to $u > u_{\rm c}$, the minus sign to $u < u_{\rm c}$, and the exponent α has to be determined numerically. As t_ξ is assumed to be the only relevant time scale, the scaling functions bridge the short time and the long time regime. To match both regimes, we require that $f_\pm(x) = {\rm const}$ for $x \ll 1$ ($t \ll t_\xi$), and $f_+(x) \sim x^{1/(d+1)-\nu_{\rm c}}$, $f_-(x) \sim x^{1/2-\nu_{\rm c}}$ for $x \gg 1$. Analogous results are expected for $g_\pm(x)$, with $g_\pm(x) = {\rm const}$ for $x \ll 1$, and $g_+(x) \sim x^{d/(d+1)-k_{\rm c}}$, $g_-(x) \sim x^{1-k_{\rm c}}$ for $x \gg 1$.

To test the scaling theory and to determine the exponent α we plotted $\langle R^2(t)\rangle/t_\xi^{2\nu_{\rm c}}$ and $\langle S(t)\rangle/t_\xi^{k_{\rm c}}$ as functions of t/t_ξ for several values of α in $d = 2$ and $d = 3$. We obtained the best data collapse for $\alpha = 5.0 \pm 0.5$ in $d = 3$ and $\alpha = 7 \pm 1$ in $d = 2$, which are shown in Fig. 3a and 3b, respectively. The excellent data collapse strongly supports the above scaling assumptions.

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[6] Note that, in the original definition by Sapozhnikov $p \sim \exp(-nu)$ with $u < 0$ [3], for convenience we use $p \sim \exp(+nu)$ with $u > 0$.

[7] The *SAW* corresponds to the case $\alpha \to -1$ and $g < 0$ of the generalized true self-avoiding walk model of Oettinger [2], where the probability p_i for moving to the neighboring site i depends on the number of previous visits n_i of site i through $p_i \sim \exp(-g\, n_i^{\alpha+1})$.

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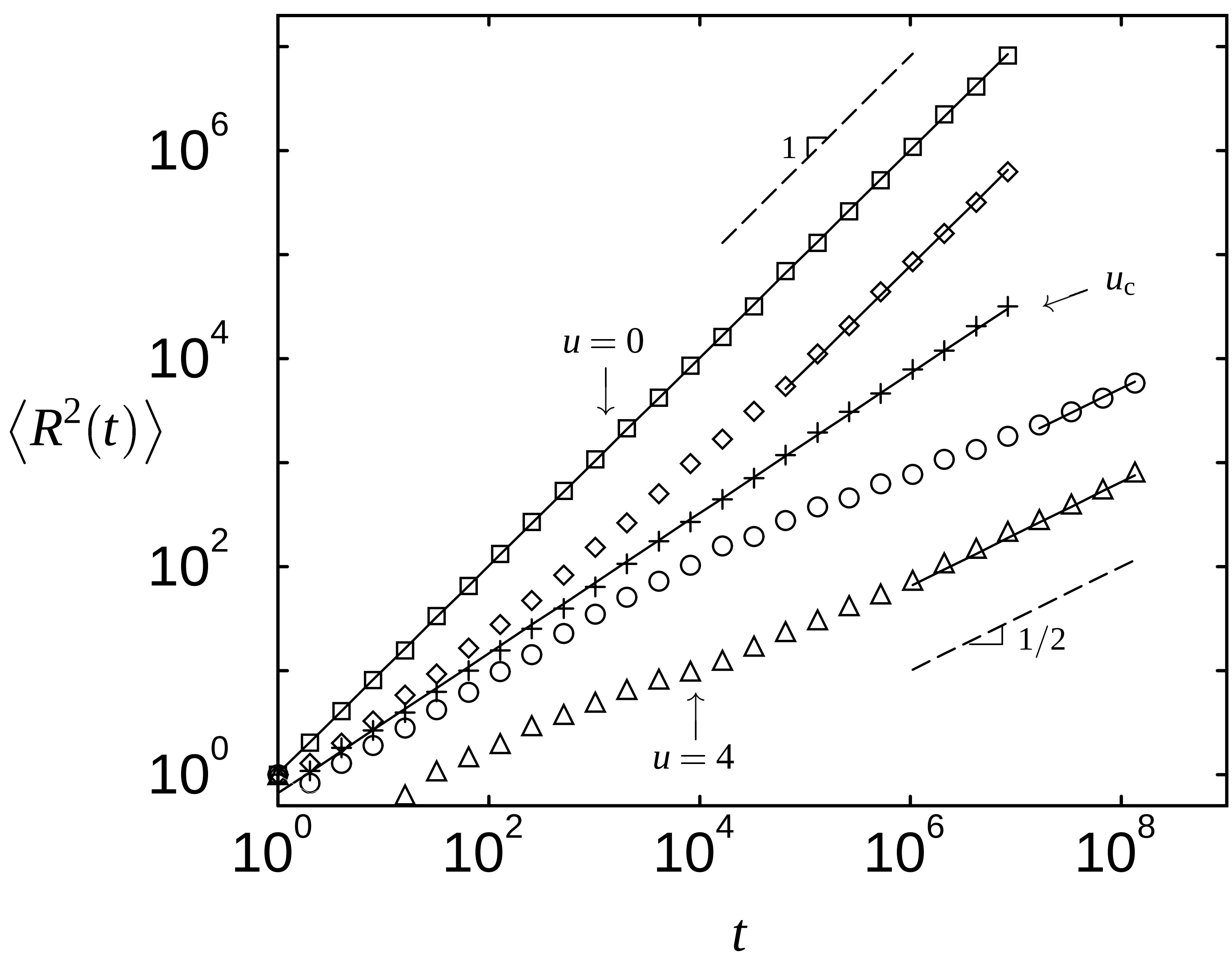
		RW			*SAW*		
		$u < u_c$	$u = u_c$	$u > u_c$	$1/T < 1/\Theta$	$1/T = 1/\Theta$	$1/T > 1/\Theta$
$d = 2$	ν	$1/2$	0.40 ± 0.01	$1/3$	$3/4$	$4/7$	$1/2$
	k	1	0.80 ± 0.01	$2/3$	1	1	1
			$u_c = 0.88 \pm 0.05$			$1/\theta_0 = 0.65 \pm 0.03$	
$d = 3$	ν	$1/2$	0.32 ± 0.01	$1/4$	0.59	$1/2$	$1/3$
	k	1	0.91 ± 0.03	$3/4$	1	1	1
			$u_c = 1.92 \pm 0.03$			$1/\theta_0 = 0.5 \pm 0.03$	

TABLE I. Comparison of the exponents ν and k as well as of the estimated values for the transition points u_c for random walks (*RW*) and Θ for *SAW* on hypercubic lattices. For values related to the Θ transition see [5] and references therein.

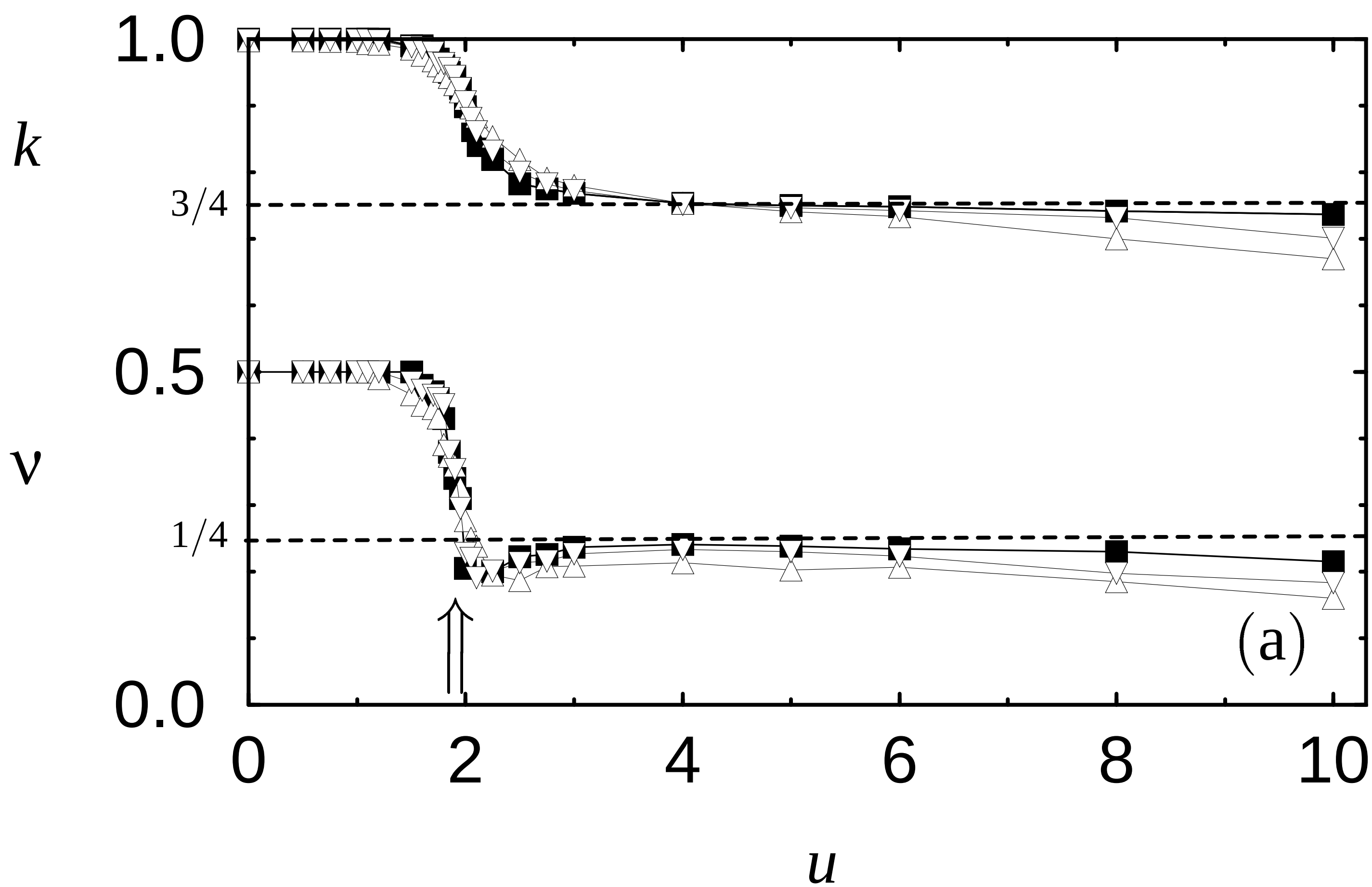
FIG. 1. The mean square end-to-end distance $\langle R^2(t)\rangle$ versus t up to $t = 10^8$ timesteps averaged over 1000 configurations for each attraction $u = 0$, 1.5, 1.9, 2.25, 4 in $d = 3$. Note that for large values of u the curves bend down towards the slope of $2\,\nu = 1/2$, while for small values of u the curves bend up towards the slope of $2\,\nu = 1$.

FIG. 2. The values of the exponents k and ν versus attraction u in (a) $d = 3$ and (b) $d = 2$, obtained by a least square fit of the slope of $\ln\langle R^2(t)\rangle$ and $\ln\langle S(t)\rangle$ versus $\ln t$ for large t, respectively (see Fig. 1). Shown are the results for $t = 10^6$ ($\triangle$), $t = 10^7$ ($\bigtriangledown$) and $t = 10^8$ ($\blacksquare$). Note that for $u > u_{\rm c}$ and larger t the values of k and ν approach the theoretical predictions of Eq. (5), marked as dashed lines. We estimate the value of $u_{\rm c}$ to be $u_{\rm c} = 1.92 \pm 0.03$ in $d = 3$ and $u_{\rm c} = 0.88 \pm 0.05$ in $d = 2$ (marked by arrows).

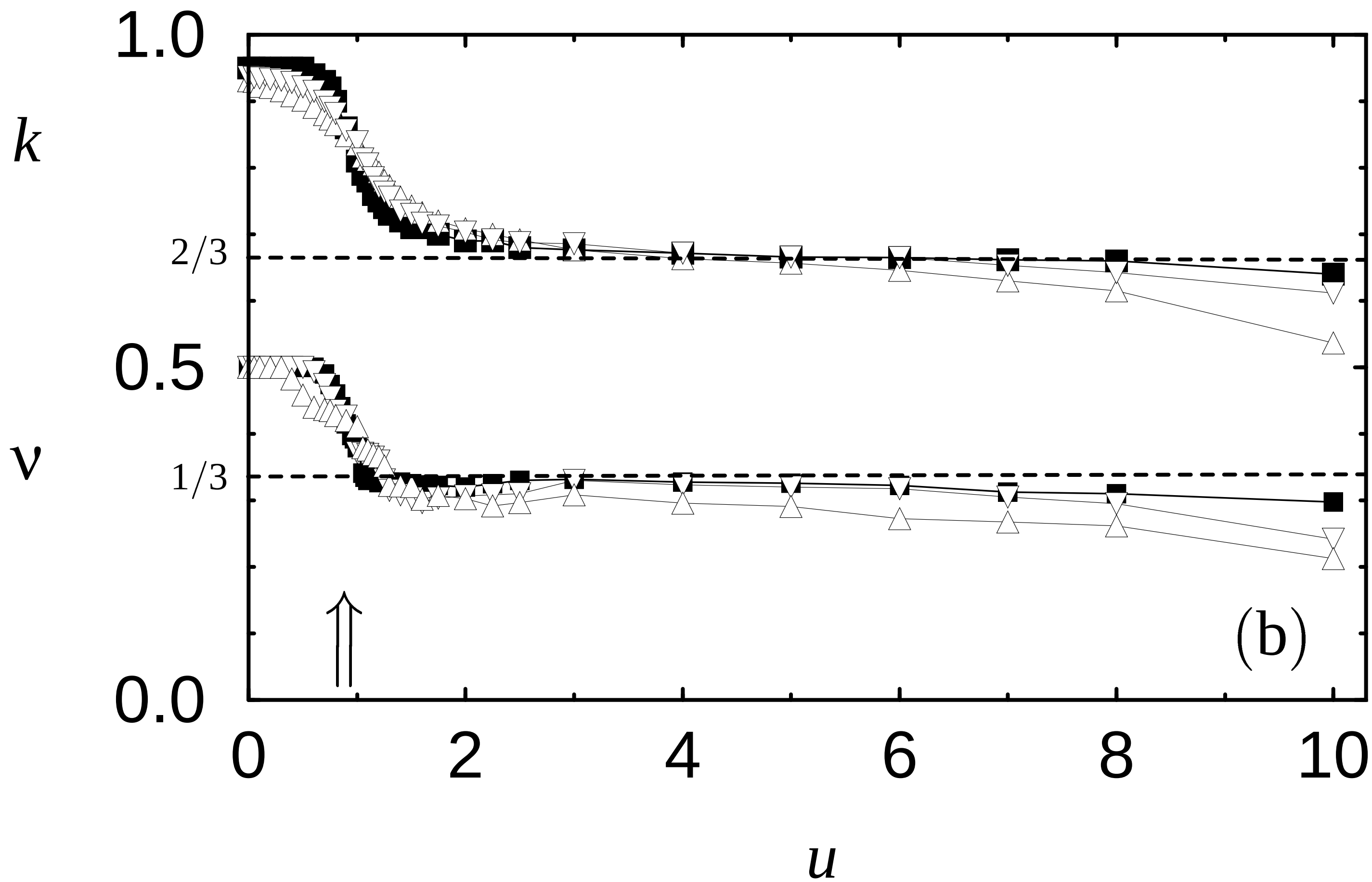
FIG. 3. Scaling plots for $\langle R^2(t)\rangle$ ($\bigcirc$) and $\langle S(t)\rangle$ ($\square$) for $t \gg 1$ and 20 values of $0 \le u \le 3$ in (a) $d = 3$ and (b) $d = 2$. For convenience, the data for $\langle S(t)\rangle$ have been shifted by 10^5. In $d = 3$ for $\nu_{\rm c} = 0.32$, $k_{\rm c} = 0.91$ and $u_{\rm c} = 1.92$ we find the best collapse for $\alpha = 5.0$, in $d = 2$ for $\nu_{\rm c} = 0.40$, $k_{\rm c} = 0.80$ and $u_{\rm c} = 0.88$ we find the best collapse for $\alpha = 7$. The straight lines represent the exponents given in Table I.



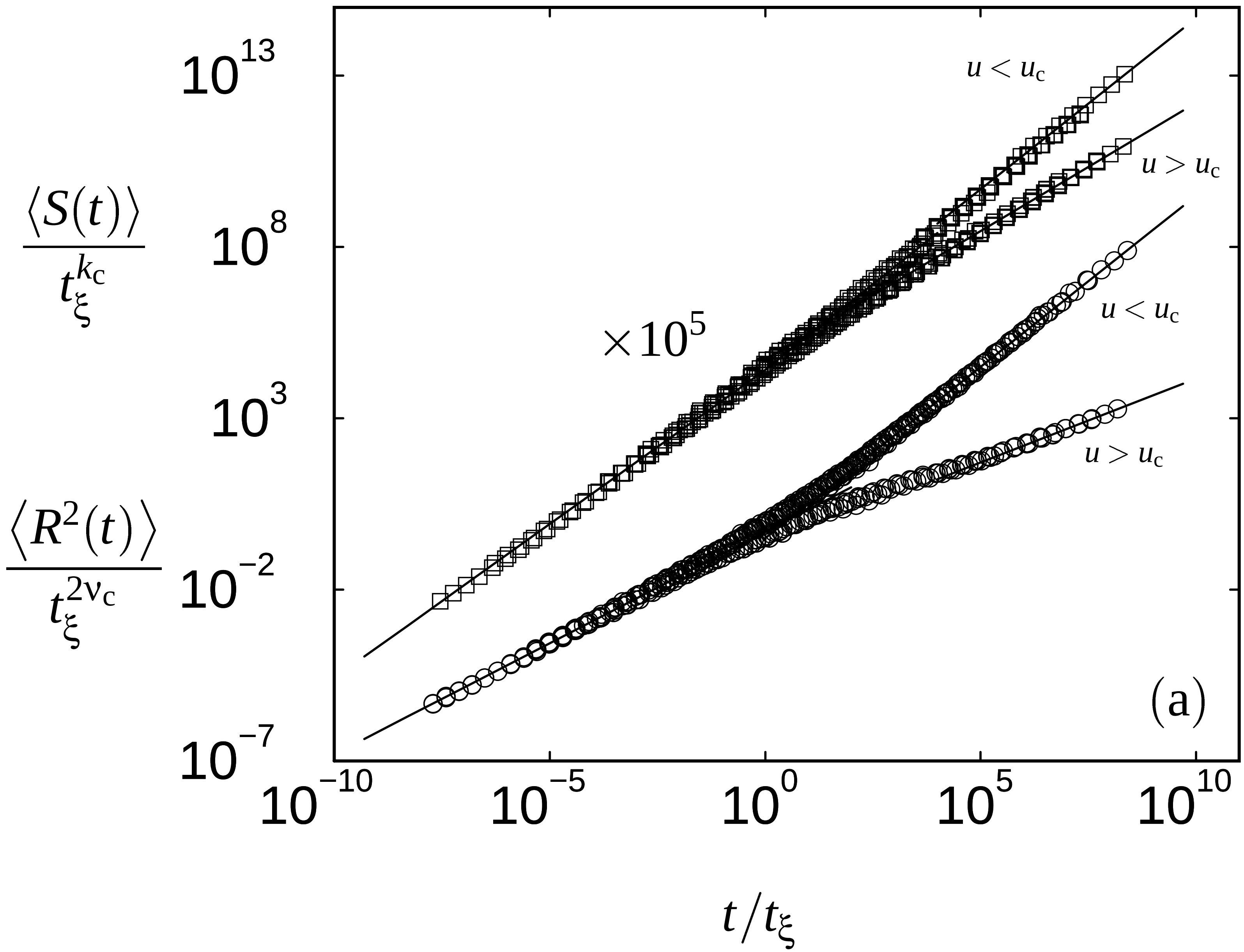
Ordemann *et al.*, Fig. 1



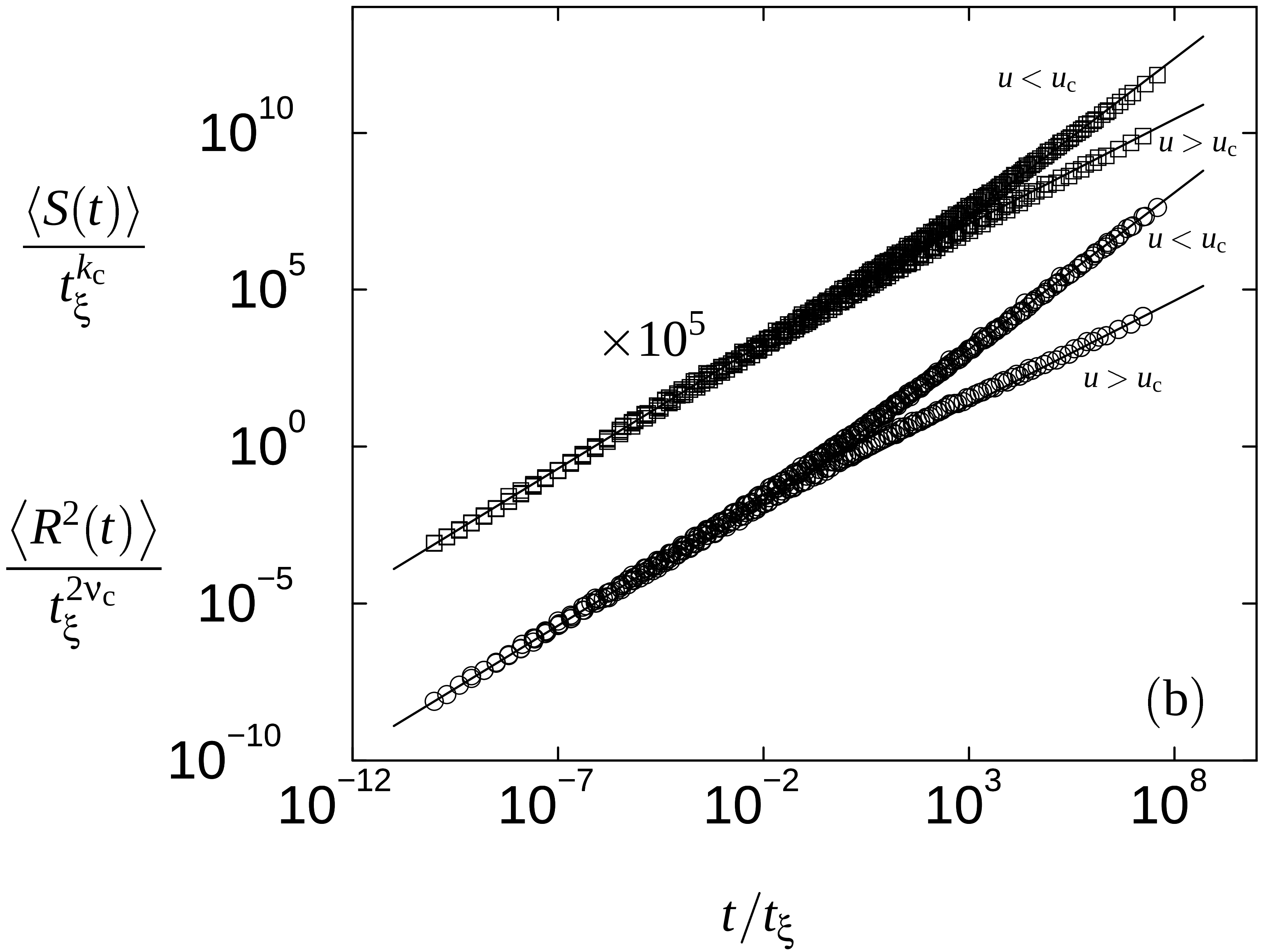
Ordemann *et al.*, Fig. 2a



Ordemann *et al.*, Fig. 2b



Ordemann *et al.*, Fig. 3a



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